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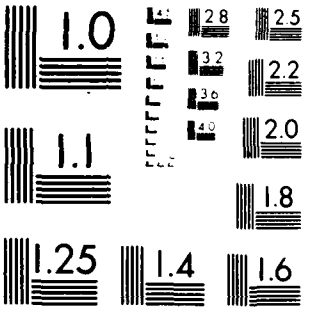

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SPECTROSCOPIC PROPERTIES OF METAL MONOXIDES AND HYDROXIDES IMPORTANT IN THE IONOSPHERE

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The $B^1\Sigma^+$-$a^3\Pi_i$ and $B'^1\Sigma^+$-$A^1\Pi$ systems of MgO have been examined by cw and pulsed dye laser fluorescence excitation spectroscopy. The B-a (0,0) and (0,1) and B-A (1,1), (2,2), and(2,1) bands have been analyzed, deperturbed, and reduced to molecular constants. The deperturbation model quantitatively accounts for the oscillator strength in the nominally forbidden $B^1\Sigma^+$-$a^3\Pi_i$ system through intensity borrowing from the $B^1\Sigma^+$-$A^1\Pi$ ($v_a \sim v_A = v_a$) and, to a lesser extent, $B^1\Sigma^+$-$X^1\Sigma^+$ ($v_a \sim v_X = v_B$) systems. A quantitative model for the v,J,Ω and

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e/f -dependence of B ← a intensity factors enables, for the first time, measurement of relative $a^3\Pi$ and $A^1\Pi$ populations from observed B → X fluorescence intensities. A significant excess population (relative to $A^1\Pi$), above the expected 500K thermal distribution is found in the e-parity levels of $a^3\Pi$ (v_a = 0 and 1) in a 1-2 Torr Mg + Ar + N_2O Broida-oven flame. Whether these e vs. f and $a^3\Pi$ vs. $A^1\Pi$ population anomalies reflect the nascent product distribution or result from complex, multiple collision processes is under investigation.

The most important use of the MgO B-a system will be proof, via OODR experiments now in progress, that the λ<320nm continuum arises from the MgO ~~$e^3\Sigma^-$ ($Mg\ ^1S + O\ ^3P$) → $a^3\Pi$~~ transition, thereby providing direct optical spectroscopic bounds to the dissociation energy of the MgO molecules.

Four papers are in preparation describing the results of this research program.

SPECTROSCOPIC PROPERTIES OF METAL MONOXIDES AND HYDROXIDES IMPORTANT IN THE IONOSPHERE

A. INTRODUCTION

The monoxides, monoxide ions, and hydroxides of Mg, Ca, and Fe are important species in the ionosphere. Spectroscopic information about these species, needed for atmospheric modelling, is either incompletely available or the subject of controversies. This program of research was originally planned to characterize the lowest lying states of MgO, CaO, and FeO and to provide a direct spectroscopic measure of the dissociation energy of MgO.

Although several projects dealing with the low lying states and electronic structure of CaO [1,2,3] and CuO[4] were completed during the period of this contract, the present report will deal exclusively with the MgO molecule.

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B. SUMMARY OF RESULTS

1. MgO $B^1\Sigma^+$-$a^3\Pi_i$ System

The $a^3\Pi_i$ state is the first excited state of MgO. It was first identified through its perturbations of the $X^1\Sigma^+$ state.[5] Although the $a^3\Pi_i$ state is an important "reservoir state" in Mg oxidation reactions and the $e^3\Sigma^-$-$a^3\Pi_i$ system has been suggested as responsible for a λ < 320nm continuum (forming Mg ^1S + O ^3P atoms)[6], no suitable scheme exists for monitoring populations in specific MgO $a^3\Pi$ rotation-vibration levels.

The main thrust of this program was to record, assign, and deperturb the MgO $B^1\Sigma^+$-$a^3\Pi_i$ intercombination system. Although nominally forbidden, the B-a system borrows oscillator strength from the $B^1\Sigma$-$A^1\Pi$ and $B^1\Sigma^+$-$X^1\Sigma^+$ systems through spin-orbit interactions of the $a^3\Pi$ state with $A^1\Pi$ and $X^1\Sigma^+$. The net result of the A~a mixing is that the $B^1\Sigma^+$-$a^3\Pi(\Omega = 1)$ sub-band is computed to have ~ 1/450 of the oscillator strength of B-A bands. However, a surprisingly large excess population in the $a^3\Pi$ e-parity levels has made recording parts of the B-a system much easier than initially expected. Unfortunately, the extremely small populations in f-parity levels and the weakness of transitions out of Ω = 0 and 2 components have made characterization of the MgO $a^3\Pi$ state unexpectedly difficult.

Table I shows the J = 0 - 50 lines of the complete B - a (0,0) band. Two complementary techniques were used: cw and pulsed dye laser fluorescence ($B^1\Sigma^+ \rightarrow X^1\Sigma^+$, Δv = 0) excitation spectroscopy (FES). The lower intensity cw laser only weakly saturates the B-A system, thus the relative B-A/B-a intensities sample populations times line strength factors. The high intensity

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TABLE 1

MgO $B^{1}\Sigma^{+}$-$a^{3}\Pi$(0,0) Observed and Calculated Line Positions (cm^{-1})[a]

J	$B-a^{3}\Pi_0$ P(J)	$B-a^{3}\Pi_0$ Q(J)	$B-a^{3}\Pi_0$ R(J)	$B-a^{3}\Pi_1$ P(J)	$B-a^{3}\Pi_1$ Q(J)	$B-a^{3}\Pi_1$ R(J)	$B-a^{3}\Pi_2$ P(J)	$B-a^{3}\Pi_2$ Q(J)	$B-a^{3}\Pi_2$ R(J)
0	-	17386.356[c]	17383.553[c]	-	-	-	-	-	-
1	17381.377[c]	386.500[c]	384.858[c]	17452.301[c]	17453.457(-7)	17455.782[c]	-	-	-
2	380.508[c]	386.788[c]	386.308[c]	451.466(11)[b]	453.785(3)	457.257(2)	17512.502[c]	17514.822[c]	17518.302[c]
3	379.783[c]	387.219[c]	387.903[c]	450.769(5)	454.259(1)	458.892(8)	511.870[c]	515.350[c]	519.990[c]
4	379.206(4)[b]	387.795[c]	389.631(-12)	450.230[c]	454.898(6)	460.669(-1)[b]	511.413[c]	516.053[c]	521.853[c]
5	378.766(-2)	388.515[c]	391.528[c]	449.849(-3)	455.695(9)	462.589(-23)[b]	511.133[c]	516.933[c]	523.893[c]
6	378.485(7)[b]	389.379[c]	393.569(12)[b]	449.631[c]	456.638[c]	464.712(2)	511.029[c]	517.989[c]	526.108[c]
7	378.328(-6)[b]	390.386[c]	395.739(7)[b]	449.573(6)	457.752(3,	466.964(-1)	511.101[c]	519.220[c]	528.499[c]
8	378.328(-7)[b]	391.539[c]	398.03(-2)[d]	449.658(-1)	459.021(2)	469.372(-4)	511.348[c]	520.627[c]	531.064[c]
9	378.485(3)[b]	392.835[c]	400.516[c]	449.910(1)	460.444(-3)	471.945(2)	511.771[c]	522.209[c]	533.805[c]
10	378.776(1)	394.276[c]	403.12[c](1)	450.312(-4)[b]	462.035(1)	474.656(-11)[b]	512.369[c]	523.967[c]	536.721[c]
11	379.206(-7)[b]	395.862[c]	405.880(-1)	450.874(-5)	463.800(9)[b]	477.548[c]	513.144[c]	525.900[c]	539.813[c]
12	379.800(3)	397.592[c]	408.784(2)	451.594(-6)	465.683(-3)	480.584(-1)	514.093[c]	529.009[c]	543.078[c]
13	380.521(-6)	399.467[c]	411.827[c]	452.481(3)	467.749(1)[b]	483.784(5)[b]	515.218[c]	530.292[c]	546.516[c]
14	381.397(-6)	401.488[c]	415.016(-3)	453.512(-2)	469.96(-1)[b,d]	487.12(-1)[d]	516.517[c]	532.750[c]	550.132[c]
15	382.432(6)	403.655(2)	418.358(3)	454.714(6)	472.348(-7)[b]	490.639(2)[b]	517.992[c]	535.382[c]	553.921[c]
16	383.591(-4)	405.973(8)	421.839(2)	456.068(9)	474.900(4)	494.301(-1)	519.641[c]	538.187(-3)	557.875(-8)
17	384.905(-6)	408.416(-5)	425.463(-2)	457.55(-2)[d]	477.601(5)	498.123(1)	521.460(-4)[b]	541.174(3)	562.012(-7)
18	386.373[c]	411.018(-6)	429.235(-4)	459.234(-1)	480.455(-1)[b]	502.101(1)	523.455(-7)	544.334(7)	566.320(-8)
19	387.972(10)	413.772(-1)	433.149(-10)[b]	461.050(-10)[b]	483.478(4)	506.237(1)	525.62(-1)[d]	547.655(-1)	570.806(-5)
20	389.72(-2)[d]	416.664(-4)	437.226(2)	463.036(-7)	486.652(1)	510.529(1)	527.984(4)	551.149(-10)	575.464(-2)
21	391 648(5)	419.718(9)	441.440(4)	465.185(1)	489.97(-2)[d]	514.983(5)	530.50(1)[d]	554.841(5)	580.294[c]
22	393.695(1)	422.898[c]	445.801(6)	467.481(-4)[b]	493.486(1,	519.588(3)	533.190(-3)	558.674(-12)[b]	585.294[c]
23	395.896(3)	426.227(-6)	450.312(13)[b]	469.96(2)[b,d]	497.139(-2)	524.36d(18)[b]	536.060[c]	562.714(5)	590.466[c]
24	398.243(3)	429.715[c]	454.952(1)	472.560(-2)	500.957(1)	529.270(-2)	539.098(-1)	566.907(3)	595.809[c]
25	400.735[c]	433.347(2)	459.750(1)	475.33(-1)[d]	504.929(-2)	534.357(5)	542.315(4)	571.282(9)	601.324[c]
26	403.381(2)	437.123(1)	464.694[c]	478.274(1)	509.060(-6)	539.594(5)	545.696[c]	575.821(8)	607.011[c]
27	406.171(1)	441.049(1)	469.78(-1)[d]	481.367(-2)	513.357(-3)	544.984(1)[b]	549.253[c]	580.526[c]	612.868[c]
28	409.114(3)	445.122[c]	475.019(-6)	484.623(1)	517.813[c]	550.536(-1)	552.988(5)	585.411[c]	618.897[c]
29	412.199(-2)	449.346(1)	480 411[c]	488.032(-4)	522.420(-7)	556.249(2)	556.886(2)	590.466[c]	625.095[c]
30	415.441(2)	453.716(-1)	485.94(-1)[d]	491.616(7)[b]	527.191(-10)	562.123(8)	560.964(7)	595.695[c]	631.463[c]
31	418.836(9)	458.240(3)	491.616(-11)[b]	495.340(-2)	532.134[c]	568.141[c]	565.201(-1)	601.094[c]	638.001[c]
32	422.365[c]	462.91(1)[d]	497.456(-1)	499.231(-3)	537.218(-9)	574.326[c]	569.622(5)	606.664[c]	644.709[c]
33	426.053(1)	467.727[c]	503.424(-10)	503.285(-1)	542.489(3)	580.668[c]	574.204[c]	612.408[c]	651.586[c]
34	429.889[c]	472.692(-4)	509.561(1)	507.492(-6)	547.899(6)	587.168[c]	578.962[c]	618.317[c]	658.632[c]
35	433.876[c]	477.818(2)	515 837(4)	511.871(1)	553.466[c]	593.826[c]	583.889[c]	624.398[c]	665.846[c]
36	438.014[c]	483.086[c]	522.254(-2)	516.401[c]	559.200[c]	600.643[c]	588.988[c]	630.654[c]	673.230[c]
37	442.302[c]	488.48(-3)[d]	528.822(-4)	521.095(2)	565.094[c]	607.617[c]	594.256[c]	637.073[c]	680.780[c]
38	446.741[c]	494.079[c]	535.548(2)	525.945[c]	571.148[c]	614.749[c]	599.695[c]	643.664[c]	688.499[c]
39	451.331[c]	499.803[c]	542.417(3)	530.959(3)	577.362[c]	622.039[c]	605.303[c]	650.425[c]	696.386[c]
40	456.072[c]	505.681(3)	549.42(-1)[d]	536.127(-1)	583.737[c]	629.487[c]	611.080[c]	657.355[c]	704.431[c]
41	460.964[c]	511.699(-6)	556.597[c]	541.457(3)	590.273[c]	637.093[c]	617.026[c]	664.454[c]	712.659[c]
42	466.008[c]	517.885(1)	563.912[c]	546.950(-1)	596.969[c]	644.855[c]	623.141[c]	671.723[c]	721.045[c]
43	471.203[c]	524.216[c]	571.374(-2)	552.600(-3)	603.825[c]	652.776[c]	629.425[c]	679.159[c]	729.596[c]
44	476.549[c]	530.705(4)	578.990[c]	558.407(-7)	610.842[c]	660.854[c]	635.876[c]	686.765[c]	738.317[c]
45	482.048[c]	537.345(6)	586.753[c]	564.384-	618.020[c]	669.089[c]	642.495[c]	694.539[c]	747.209[c]
46	487.698[c]	544.130[c]	594.664[c]	570.506(-9.	625.358[c]	677.480[c]	649.291[c]	702.480[c]	756.247[c]
47	493.500[c]	551.072(-2)	602.726[c]	576.803[c]	632.857[c]	686.029[c]	656.232[c]	710.569[c]	765.456[c]
48	499.454[c]	558.175(3)	610.937[c]	583.249[c]	640.518[c]	694.732[c]	663.349[c]	718.867[c]	774.832[c]
49	505.560[c]	565.425[c]	619.297[c]	589.855[c]	648.339[c]	703.592[c]	670.629[c]	727.312[c]	784.366[c]
50	511.819[c]	572.832[c]	627.806[c]	596.617[c]	656.322[c]	712.605[c]	678.070[c]	735.929[c]	794.056[c]

a Number in parentheses is (observed - calc.) in 10^{-2} cm^{-1}.
b Blended lines.
c Calculated lines.
d These lines are obtained by using a pressure-scanned pulsed dye laser with a HWHM of 0.02cm^{-1}. Experimental uncertainties for these lines are 0.04cm^{-1}.

TABLE II

Constants for the a, B, and X States of MgO (cm^{-1})[a]

	$a^3\Pi$		$B^1\Sigma^+$	$X^1\Sigma^+$		
	v = 0	v = 1[b]	v = 0	v = 0	v = 3	v = 4
T_o	2553.755(19)	3195.4625(16)	20003.575(11)	0.0[d]	2293.67(43)	3038.54(46)
B_v	0.500341(12)	0.495556(7)	0.580058(12)	0.571987(25)	0.5568[c]	0.55151(19)
$D_v \times 10^6$	1.1979(49)	1.1072(40)	1.1485(47)	1.2173(97)	1.29[c]	1.31[c]
A_v	-63.489(14)	-64.1727(73)	-	-	-	-
$A_{D_v} \times 10^4$	-1.214(27)	-2.953(80)	-	-	-	-
A_{01}	17.69(27)	20.889(29)	-	-	-	-
A_{11}	-65.11(11)	-64.85[c]	-	-	-	-
O_v	-1.046(28)	-0.619[c]	-	-	-	-
P_v	-0.02001(25)	0.02391(36)	-	-	-	-
$q_v \times 10^4$	-0.96(10)	-1.96[c]	-	-	-	-
$O_{D_v} \times 10^4$	-0.741(88)	-	-	-	-	-

a Number in parentheses is one standard deviation uncertainty.
b Preliminary values. Constants for $B^1\Sigma^+$ were fixed.
c Held fixed in the fit.
d Zero of energy.

pulsed laser saturates both transitions, hence sampling relative populations. Although B-a lines are weaker than B-A in the cw laser spectra, the B-A lines are barely detectable in the pulsed laser spectra! The use of pulsed laser FES will provide the crucial missing Ω = 0 and 2 lines in the B-a (0,1) band.

Table II gives the constants for the $a^3\Pi$ v = 0 and 1 levels obtained from the measured lines of the B-a (0,0) and (0,1) bands. Reduction to a set of mechanically and magnetically meaningful constants required deperturbation of $a^3\Pi$ v_a with respect to interactions with $X^1\Sigma^+$ $v_X = v_a + 3$ and $A^1\Pi$ $v_A = v_a$. In turn this deperturbation model yields precise basis function mixing coefficients which enable calculation of v,J, Ω, and e/f dependent B-a intensity factors.

2. Intensities in the MgO $B^1\Sigma^+$-$a^3\Pi_i$ System

In order to make quantitative measurements of the relative populations of $a^3\Pi_\Omega$ e vs. f, $a^3\Pi_\Omega$ vs $a^3\Pi_{\Omega\pm1}$, or $a^3\Pi_\Omega$ vs $A^1\Pi$ levels, it is necessary to know the relative linestrength factors. Such factors are never trivially available for a nominally forbidden band system. Fortunately, the B ← a (v_B,v_a) band of the FES spectrum monitored by B → X (v_B,$v_X = v_B$) fluorescence, borrows more than 99% of its intensity from the B-A (v_B, $v_A = v_a$) band. This means that knowledge of the $A^1\Pi$ character in each nominal $a^3\Pi$ v_a,J,Ω, e/f level is sufficient to calculate the intensity of any B-a line relative to any B-A or other B-a line. The $A^1\Pi$ fractional character varies over several orders of magnitude, and the mixing fractions obtained from the deperturbation model are accurate to better than 1% of their calculated magnitudes. The deperturbation model yields mixing fractions which should be considerably more accurate than state-of-the-art absolute intensity measurements.

Although unimportant for most purposes, quantum mechanical interferences between B-A and B-X transition amplitudes can cause certain B-a lines to behave anomalously. P and R lines from a common J" level would normally have comparable linestrengths. However, for B ← a bands detected by B → X $\Delta v \neq 0$ fluorescence, the P/R intensity ratio will deviate significantly from 1. Whether it is greater or less than 1 determines the relative signs of the B - X and B - A transition moments.

For the first time, populations in the most important "reservoir state" of MgO, the MgO $a^3\Pi$ state, can be monitored systematically and without assignment ambiguity. The monitoring transition is in the convenient Rhodamine 6-G region and had the simplest possible branch structure. Although

the d-a system has been used for monitoring $a^3\Pi$, its complex structure has, to date, frustrated analysis. The availability of $a^3\Pi$ combination differences should facilitate assignment of the $d^3\Delta$-$a^3\Pi$ system and resolution of several contradictory features of speculative bandhead assignments.[5,7]

3. Relative $a^3\Pi e/a^3\Pi f$ and $a^3\Pi/A^1\Pi$ Populations.

Armed with the calculated linestrength factors from the $a^3\Pi \sim A^1\Pi$, $X^1\Sigma^+$ deperturbation, it becomes possible to measure population ratios and to compare these ratios to those expected from a thermal ($T \tilde{\sim} 500K$) distribution. At 1-2 Torr total pressure (99% Ar, 1% N_2O, 0.1% MgO and Mg), it is reasonable to expect the metastable X,A, and a levels to to be equilibrated. However, the $a^3\Pi$ $v = 0$, $\Omega = 1$ levels have more than a factor of 10 higher population relative to $A^1\Pi$ $v = 0$ than the 950 cm^{-1} separation of these levels would imply at 500K. Similarly, the $a^3\Pi$ $\Omega = 1$ e-levels have more than a factor of 2 greater population than the near degenerate ($\Delta E < 0.1$ cm^{-1}) f-levels. It is difficult to imagine how such large departures from equilibrium could exist at such high pressure.

Single collision Mg $+N_2O$ experiments, in collaboration with Professor Paul Dagdigian at Johns Hopkins University, are in progress. The purpose of these experiments is to determine whether the 1-2 Torr population anomalies reflect nascent product distributions or complex multiple-collision population funnelling and removal processes.

4. Dissociation Energy of MgO

Ground state Mg and O atoms correlate adiabatically with the MgO $a^3\Pi$ and $e^3\Sigma^-$ states. The e-a transition is predicted to be strong because the $e^3\Sigma^-$ state belongs to the same electronic configuration as $d^3\Delta$, $D^1\Delta$, and $C^1\Sigma^-$. Evans and Mackie[6] have observed a continuum in absorption from shock-heated MgO at $\lambda < 320$ nm which they have assigned as $e^3\Sigma^- \leftarrow a^3\Pi$. If this assignment can be verified and the long-λ limit of the continuum can be located with greater sensitivity, it should be possible to obtain a direct spectroscopic upper bound to D_0° (MgO).

Our initial purpose for investigating the MgO B-a system was to develop and unambiguous $a^3\Pi$ population monitor for use in an Optical-Optical Double Resonance (OODR) scheme for assigning and extending the Evans-Mackie continuum. Laser 1 destroys MgO $a^3\Pi$ by pumping in the continuum. Laser 2 detects MgO $a^3\Pi$ and shows that the population destruction which occurs when Laser 1 pumps in the continuum is specific to $a^3\Pi$ $v = 0$. If the Evans-Mackie assignment is correct, then population loss in $A^1\Pi$ (monitored by Laser 2 in the B-A system) will occur at a longer delay after the Laser 1 pulse than population loss in $a^3\Pi$.

The pulsed laser FES component of this experiment has been demonstrated. The full OODR experiment will be performed in March, 1983.

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PERSONNEL

1. Visiting Scientists

   Dr. Richard F. Barrow, Oxford University

   Dr. Bernard Bourguignon, Paris-Sud (Orsay)

   Dr. Guy Taieb, Paris-Sud (Orsay)

2. Postdoctorals

   Dr. Keith J. Cross (cw MgO B-a)

   Dr. Carter Kittrell (pulsed MgO B-a)

   Dr. Hartmut Schweda

3. Graduate Students

   Evan Abramson

   Stewart Cameron (pulsed MgO B-a)

   Michael Dulick (consultant)
   Ph.D., May 1982

   Jeffrey Gray (pulsed MgO B-a)

   Precila Ip (cw and pulsed MgO, major participant)
   Ph.D., June 1983 (expected)

   Jeffrey Norman (pulsed MgO B-a)

   David E. Reisner
   Ph.D., March 1983 (expected)

PUBLICATIONS

The following papers are in preparation:

1. Precila C.F. Ip, Robert W. Field, and Keith J. Cross, "The $B^1\Sigma^+$-$a^3\Pi_i$ Intercombination System of the MgO Molecule," for J. Mol. Spectrosc.

2. Keith J. Cross and Precila C.F. Ip, "The MgO $B^1\Sigma^+$-$A^1\Pi$ System. Laser Spectroscopy and Deperturbation," for J. Mol. Spectrosc.

3. Precila C.F. Ip and Robert W. Field, "Intensity Factors for the MgO $B^1\Sigma^+$-$a^3\Pi_i$ System Based on $X^1\Sigma^+$~$a^3\Pi_i$~$A^1\Pi$ Deperturbation Model," for Chem. Phys. Lett.

4. Precila C.F. Ip, Keith J. Cross, and R.W. Field, "Population Anomalies in an Mg+N_2O Flame. Excess $a^3\Pi/A^1\Pi$ and $a^3\Pi_e/a^3\Pi_f$ Populations," for J. Phys. Chem.

INTERACTIONS AND PRESENTATIONS

6-80 Molecular Spectroscopy Symposium, Columbus, Ohio, P.F. Bernath, P. Ip, and R.W. Field, "Optical-Optical Double Resonance Spectroscopy of BaF" (contributed talk MF5).

3-81 Yale University, Symposium on Lasers in Chemistry, R.W. Field, "Molecular Spectroscopy Beyond Molecular Constants" (invited).

4-81 Discussion of Faraday Society, No. 71, Bristol, England, R.W. Field, "Tunable Laser Electronic Spectroscopy" (invited).

5-81 International Colloquium on Molecular Spectroscopy, Stockholm, Sweden, R.W. Field, "Perturbations: Sublime and Ridiculous" (invited).

6-81 Molecular Spectroscopy Symposium, Columbus, Ohio, K.J. Cross, P. Ip, and R.W. Field, "Rotational Analysis of the $B^1\Sigma^+$-$a^3\Pi_i$ Band System of MgO (contributed talk MG7).

3-82 Bad Honnef, Germany, conference of the Deutsche Bunsengesellschaft für Physikalische Chemie on Small Molecules in the Gas Phase, R.W. Field, "Electronic Structure of Diatomic Molecules Beyond Simple Molecular Constants" (invited).

8-82 Gordon Conference on Molecular Electronic Spectroscopy, R.W. Field, "The Electronic Structure of Ionic Diatomic Molecules" (invited).

Collaborations with Dr. Guy Taieb and Dr. Bernard Bourguignon at Université de Paris-Sud, Orsay and Professors Yarkony and Dagdigian at Johns Hopkins University.